

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.25e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.05e-01

Confidence level: 5.01e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Niclosamide</div> <div>Measured: 1.49e-11</div> <div>Predicted: 2.02e-11</div>	<div>Image not found</div> <div>Butanedinitrile, ethyl-</div> <div>Measured: 3.70e-09</div> <div>Predicted: 1.62e-02</div>	<div>Image not found</div> <div>Oct-2-yne</div> <div>Measured: 5.00e-11</div> <div>Predicted: 10.3</div>
<div>Image not found</div> <div>3-Methyl-N-phenylaniline</div> <div>Measured: 1.79e-11</div> <div>Predicted: 1.24e-04</div>	<div>Image not found</div> <div>Acetone</div> <div>Measured: 8.76e-10</div> <div>Predicted: 262</div>	